Machine Learning 1

Lecture 4.1 - Supervised Learning
Model Selection

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(Bishop 1.3)

Slide credits: Rianne van den Berg

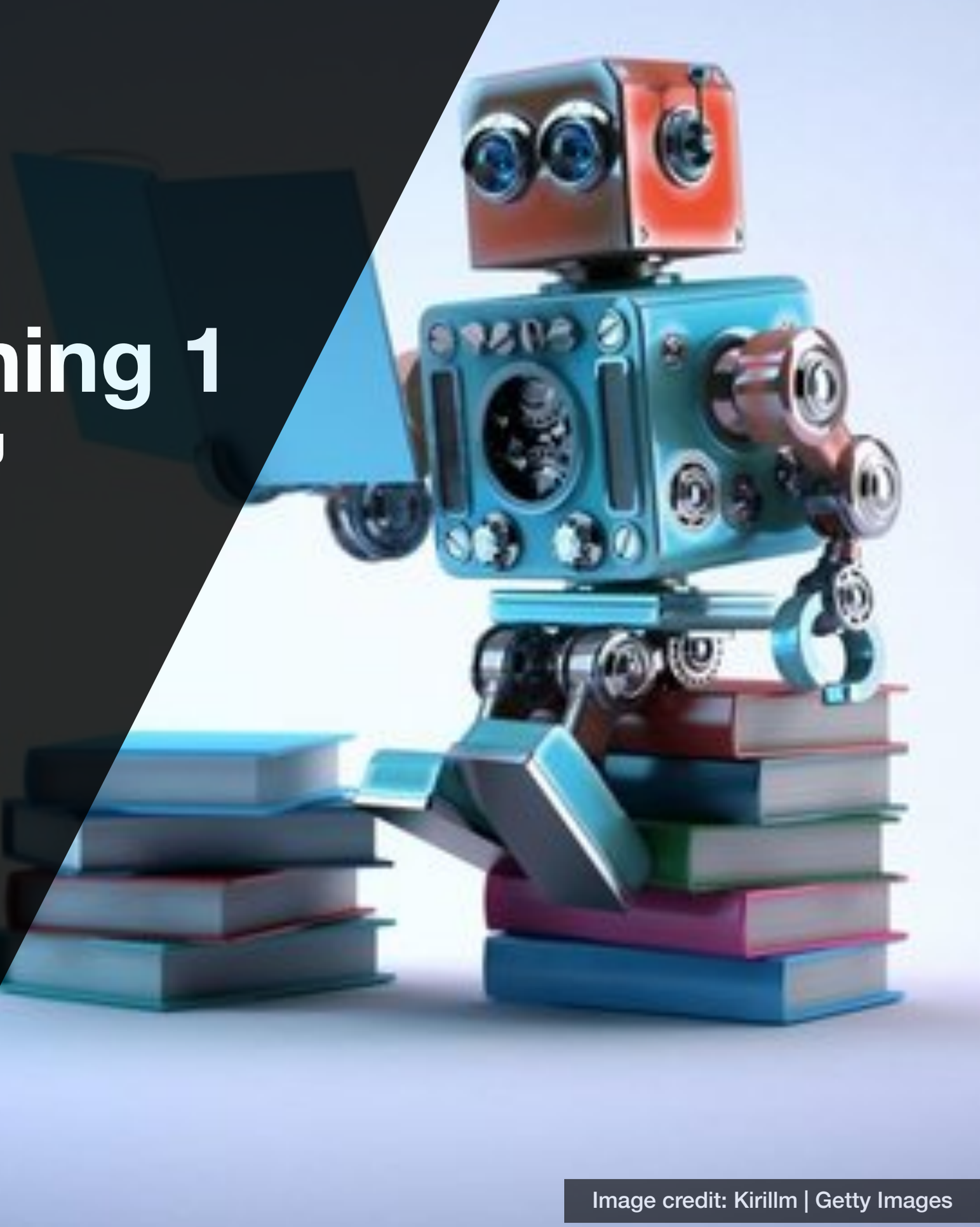


Image credit: Kirillm | Getty Images

Supervised Learning: Evaluating Errors

Question 1:

How can we estimate the model performance properly for unknown data?

Question 2:

How can we choose the optimal hyperparameters?

Supervised Learning: Evaluating Errors

Solution

Divide data $D = \{(\mathbf{x}_1, t_1), ..., (\mathbf{x}_N, t_N)\}$ in 3 groups:

- Training set D_{train} (± 80 % of D):
  - Minimize the error $E(y(x), t)$ for $(\mathbf{x}, t) \in D_{\text{train}}$ → $\mathbf{w}^*$
- Validation set D_{val} (± 10 % of D):
  - Used to estimate test error $E(y(\mathbf{x}_{\text{val}}, \mathbf{w}^*), t_{\text{val}})$
- Test set D_{test} (± 10 % of D):
  - final test/generalization error estimate $E(y(\mathbf{x}_{\text{test}}, \mathbf{w}^*), t_{\text{test}})$

repeat for different hyper-parameter settings

model selection part

Can never be part of model selection!!!

Supervised Learning: Small Datasets

- Small dataset → small validation and test set
- Approximate validation step!

Cross-validation

- Split data: $D = \{(x_1, t_1), ..., (x_N, t_N)\}$ into K-folds
- Train *y* on *K-1* folds $\hat{y}^{-k}(x)$

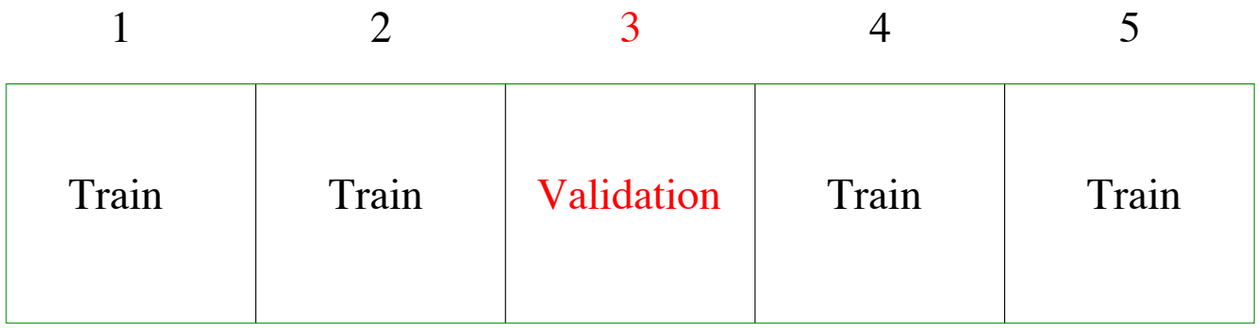


Figure: K-fold splitting of dataset (ESL 7.10)

- $K = N$: leave-one-out cross validation

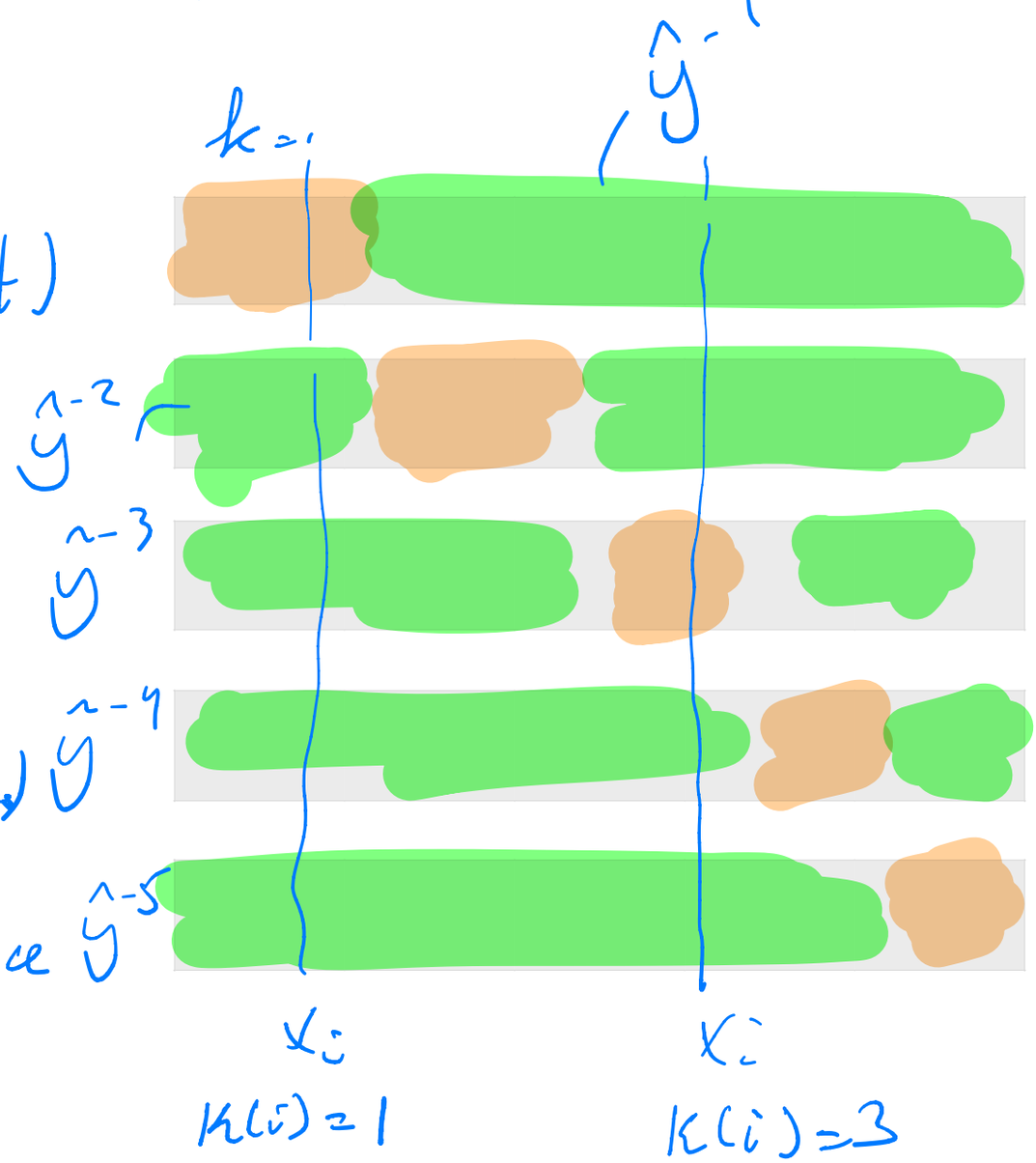
Cross-Validation

- *K* trained functions $\hat{y}^{-k}(x)$
- Indexing function $\kappa : \{1, ..., N\} \mapsto \{1, \ldots, K\}$
- Estimate of prediction error

$$CV(\hat{y}) = \frac{1}{N} \sum_{i=1}^{N} L(y_i, \hat{y}^{-\kappa(i)}(x_i))$$

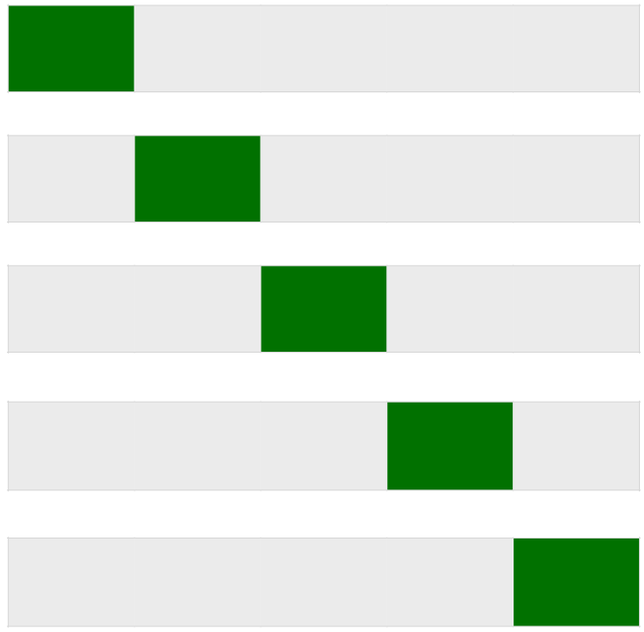
2 tasks

1. model selection (optimal hyperparameter)
2. estimate model performance



Cross-Validation: Model Selection

- Hyperparameter selection α
- $CV(\hat{y}_\alpha) = \frac{1}{N} \sum_{n=1}^{N} L(\hat{y}_\alpha^{(k(n))}(x_n), t_n)$
- Optimal $\alpha^* = \arg\min_\alpha CV(\hat{y}_\alpha)$



- Multiple hyperparameters: $\alpha \in \{\alpha_1, \alpha_2\}$, $\beta \in \{\beta_1, \beta_2, \beta_3\}$
  - How many times should CV be performed?

    2×3
  - Total number of training runs?

    $6K$

Cross-Validation: Test Error Estimation

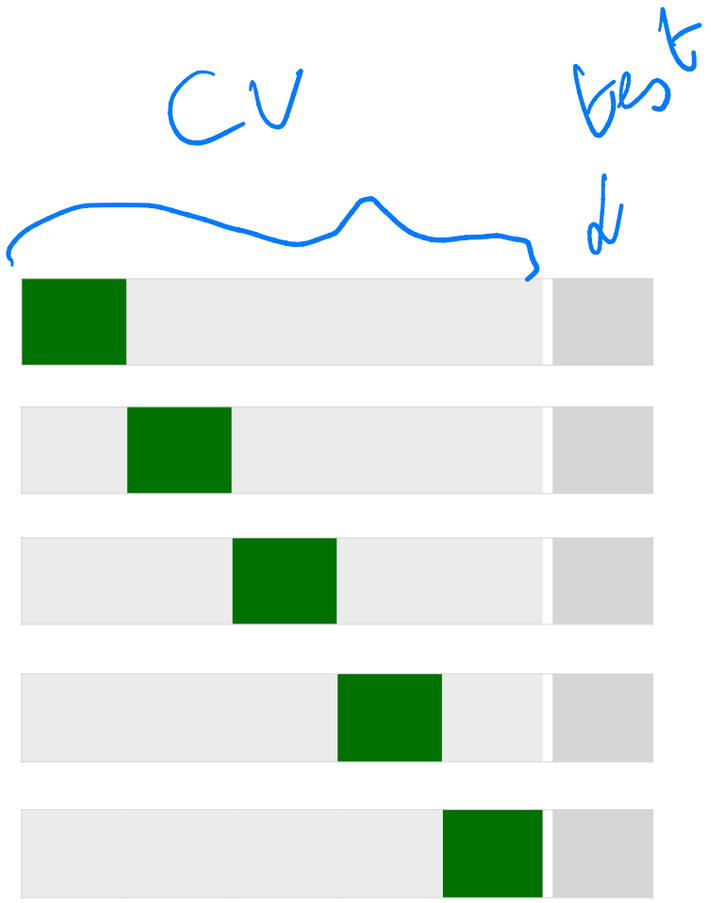
- After Model selection

$$\alpha^*, \beta^*$$

- Retrain *f* on all K folds with α^*, β^*

- Evaluate model on held-out test set

- Nested cross validation!



Nested Cross-Validation

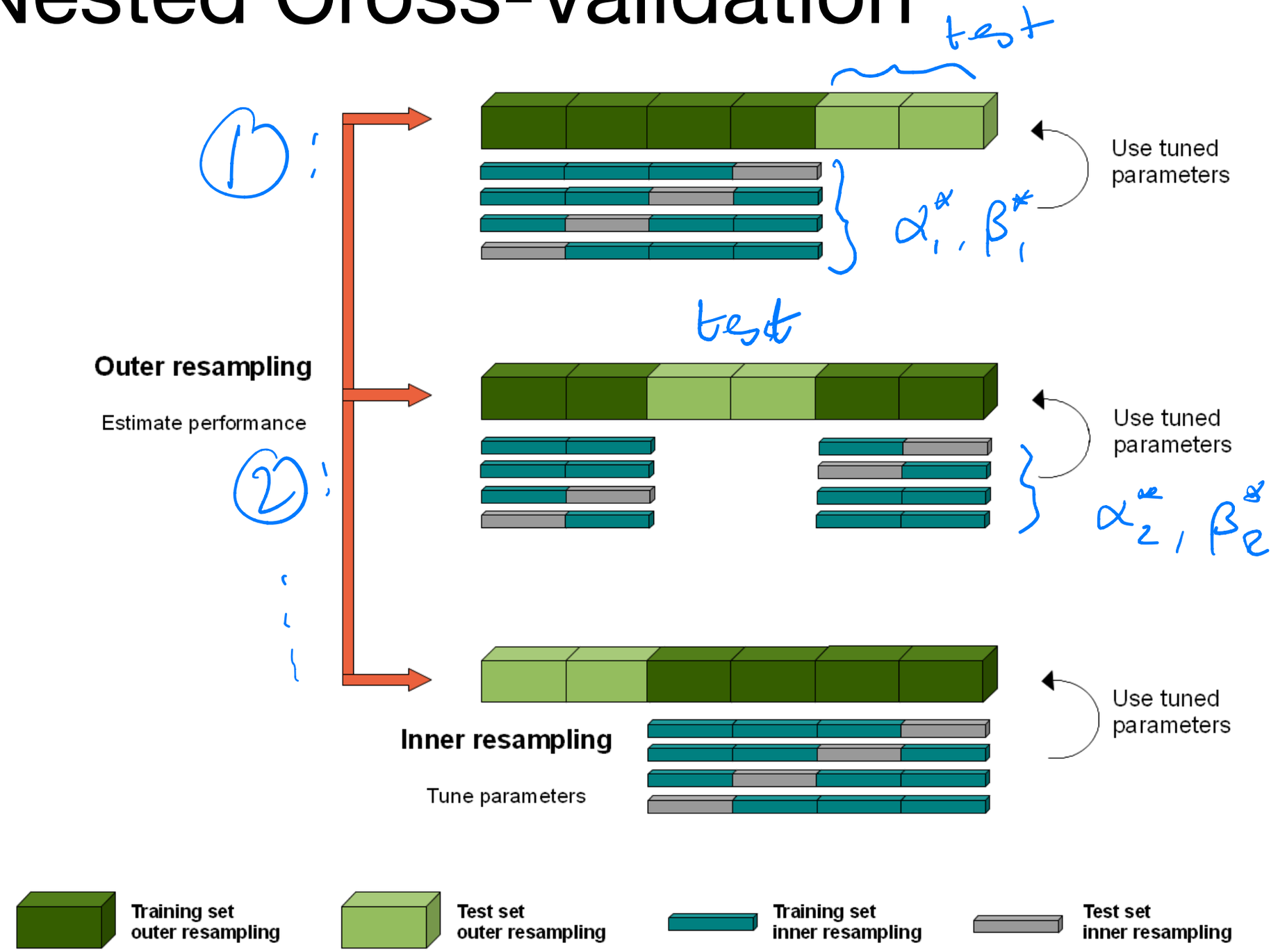


Figure: Nested cross-validation
https://mlr-org.github.io/mlr-tutorial/devel/html/nested_resampling/index.html